2-Ethyl-p-xylene 1758-88-9 | DTXSID0061951

Model Performance

Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.81	0.55	0.81	0.54	0.71	0.61	

Model Results

Predicted value: 738 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.30e-01

Confidence level: 5.81e-01

Nearest Neighbors from the Training Set

Image not found

1,2,4,5-Tetramethylbenzene

Measured: 1320 Predicted: 1510

Image not found

2,3,5-Trimethylphenol

Measured: 4070 Predicted: 345

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Propylbenzene Measured: 741 Predicted: 859

Image not found

Isophorone
Measured: 25.1
Predicted: 103

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1,2,3-Trimethylbenzene

Measured: 631 Predicted: 691